

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 162401-32-3 REGISTRY
 ED Entered STN: 21 Apr 1995
 CN Benzamide, 3-(cyclopropylmethoxy)-N-(3,5-dichloro-4-pyridinyl)-4-(difluoromethoxy)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN B 9302-107

CN BY 217

CN BYK 20869

CN Roflumilast

FS 3D CONCORD

MF C17 H14 Cl2 F2 N2 O3

CI COM

SR CA

LC STN Files: ADISINSIGHT, ADISNEWS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MRCK*, PHAR, PROMT, PROUSDDR, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
 (*File contains numerically searchable property data)

DT.CA CAplus document type: Dissertation; Journal; Patent

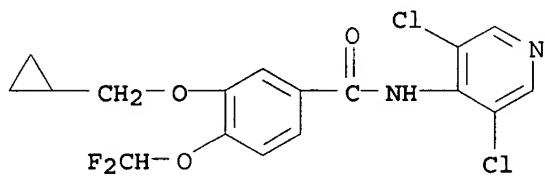
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID	Occurrence Count
EA	ES	SZ	RF	RID		
C3	C3	3	C3	1.13.1	1	
C6	C6	6	C6	46.150.18	1	
C5N	NC5	6	C5N	46.156.30	1	



Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	NOTE
Melting Point (MP)	157-157.5 deg C	(1) CAS

(1) Williams, Eric L.; WO 2004033430 A2 2004 CAPLUS

Experimental Property Tags (ETAG)

PROPERTY	NOTE

Crystal Structure | (1) CAS

(1) Card, Graeme L.; Structure (Cambridge, MA, United States) 2004 V12(12)
P2233-2247 CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1467.15	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	2550.56	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	2754.55	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	2776.77	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	2778.97	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	2778.88	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	2775.70	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	2744.04	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	2463.46	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1225.92	pH 10 25 deg C	(1)
Boiling Point (BP)	430.6+/-45.0 deg C	760 Torr	(1)
Density (DEN)	1.471+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	68.60+/-3.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	214.2+/-28.7 deg C		(1)
Freely Rotatable Bonds (FRB)	7		(1)
H acceptors (HAC)	5		(1)
H donors (HD)	1		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	6		(1)
Koc (KOC)	5358.28	pH 1 25 deg C	(1)
Koc (KOC)	9315.11	pH 2 25 deg C	(1)
Koc (KOC)	10060.14	pH 3 25 deg C	(1)
Koc (KOC)	10141.26	pH 4 25 deg C	(1)
Koc (KOC)	10149.33	pH 5 25 deg C	(1)
Koc (KOC)	10148.97	pH 6 25 deg C	(1)
Koc (KOC)	10137.34	pH 7 25 deg C	(1)
Koc (KOC)	10021.74	pH 8 25 deg C	(1)
Koc (KOC)	8997.00	pH 9 25 deg C	(1)
Koc (KOC)	4477.27	pH 10 25 deg C	(1)
logD (LOGD)	4.56	pH 1 25 deg C	(1)
logD (LOGD)	4.80	pH 2 25 deg C	(1)
logD (LOGD)	4.83	pH 3 25 deg C	(1)
logD (LOGD)	4.83	pH 4 25 deg C	(1)
logD (LOGD)	4.83	pH 5 25 deg C	(1)
logD (LOGD)	4.83	pH 6 25 deg C	(1)
logD (LOGD)	4.83	pH 7 25 deg C	(1)
logD (LOGD)	4.83	pH 8 25 deg C	(1)
logD (LOGD)	4.78	pH 9 25 deg C	(1)
logD (LOGD)	4.48	pH 10 25 deg C	(1)
logP (LOGP)	4.835+/-0.726	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.00089 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0017 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00097 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00097 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0020 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00089 g/L	Unbuffered Water	(1)
		pH 6.99	

Molar Intrinsic Solubility (ISLB.MOL)	0.0000022 mol/L	25 deg C 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000041 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000024 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000024 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000049 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000022 mol/L	Unbuffered Water pH 6.99	(1)
Molar Volume (MVOL)	273.9+/-3.0 cm**3/mol	25 deg C 20 deg C 760 Torr	(1)
Molecular Weight (MW)	403.21		(1)
pKa (PKA)	9.89+/-0.70	Most Acidic	(1)
pKa (PKA)	0.95+/-0.46	25 deg C Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	60.45 A**2		(1)
Vapor Pressure (VP)	1.28E-07 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14
 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

118 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

118 REFERENCES IN FILE CAPLUS (1907 TO DATE)